FINAL

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DOE/NNSA Advanced Simulation and Computing

Predictive Science Academic Alliance Program (PSAAP)

Procurement Department
(University of California/DOE/NNSA, Contract W-7405-ENG-48)
Department of Energy/National Nuclear Security Administration

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May 26, 2006

Request For Expression of Interest and Preliminary Proposals for ASC Multidisciplinary Simulation Centers

Dear Colleague:

The National Nuclear Security Administration (NNSA) Office of Advanced Simulation and Computing (ASC), with Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL), is initiating the next phase of its academic computational science program. The vision for the next ASC Alliance program phase, called Predictive Science Academic Alliance Program (PSAAP), includes participation by leading universities to establish validated, large-scale, multidisciplinary, simulation-based "Predictive Science" as an accepted academic and applied research programs as further described by the "PSAAP Program Statement" and other Internet accessible information at **http://www.llnl.gov/asci/alliances/psaap/**. LLNL, which is charged with contractually administering the PSAAP, is issuing this Request as an invitation for your institution to submit an expression of interest and preliminary proposal in accordance with the guidelines stated herein.

The current PSAAP program is anticipated to consist of the following:

Multidiscipline Simulation Centers (MSCs) - centers whose research will focus on large-scale, multidisciplinary, scalable and integrated simulations to be carried out on massively parallel ASC systems. Each Center has the primary goal to develop a verified and validated, predictive capability for their specific application. They are broad in discipline and focused in application and must develop a technical and sociological framework that allows each component (discipline) to be effectively integrated into the whole. Further, significant depth in each scientific component must exist in the resulting simulations to provide for meaningful verified, validated, predictive simulation experiments to be performed to demonstrate large-scale predictive science. This type of Center is motivated by the need to demonstrate predictive science in highly visible unclassified ASC-class problems, to develop the multidiscipline predictive science methodology, and to establish training and education programs in this new science area. As guidelines, the selected MSCs' funding will ramp up to approximately $4M per year for up to five years.

Collaborating Research Activities (CRAs) - In order to expand the number of universities involved, to increase the visibility of the program, and to bring unique research capabilities into the program (variable over the life of PSAAP), a portion of the ASC Alliance budget will be set aside for smaller efforts directly integrated with one or more MSCs and the NNSA Laboratories. Such efforts will fall into the range of $200-800K per year, for up to 3 years, and cover topics such as experiments, models, tools, algorithms, etc. Each activity will likely involve only a single site. Such activities could span MSCs and NNSA Laboratories, helping to form tighter relationships and sharing of common approaches. Thus the goal is not only to simply broaden the number of universities involved in the program, but also to encourage broadening the web of relationships and collaborations that might continue under other funding mechanisms later. All such efforts will have to be endorsed by each of the Centers to which the effort will be tied, and meet the criteria of NNSA Laboratory relevance and integration. Competition for these awards will occur roughly every two to three years beginning in the second year of the program. Such a schedule will allow for flexibility in targeting technical areas that need research attention and assistance from the academic community.

This Request for Expression of Interest and Preliminary Proposals is for the MSCs only. The call for proposals for the CRAs will take place in FY08, after the awards of the MSC's are announced and if programmatic funding permits.

Expressions of interest and preliminary proposals for the MSCs must be received at LLNL by **July 17, 2006** in order to receive consideration. Preliminary proposals received after this date may not be accepted. Acceptance of late submissions will be at the sole discretion of LLNL. If proprietary data is included in the preliminary proposal, it must be marked "Proprietary" and best effort will be exercised to avoid disclosure of such data to the general public.

NOTE: As a result of the Dallas May 16-17, 2006 Bidders Meeting, we've made an important change to the submission rule. A university can submit more than one preliminary proposal, provided that it meets all of the following conditions:

- **Each submission must have a different PI.**
- **Each submission must target a significantly different application.**
- **There must be no overlap of personnel in the application area of interest.**
- **The Vice President for Research, or someone in a comparable position, must include a letter acknowledging the preliminary proposal submission.**

NOTE: Only one full proposal per university campus will be accepted in response to the RFP that will be issued in mid September 2006.

Preliminary proposals should focus on the establishment of a validated, large-scale, multidisciplinary, simulation-based "Predictive Science" academic and applied research program. Be specific, concise and include the following information (font size should not be smaller than 11):

(1) A one-page executive summary of the approach and tasks proposed for the Center.

(2) No more than seven pages describing the technical and scientific approaches and objectives for the work, with an outline plan that presents the multidisciplinary simulation of a large, complex problem of ASC and national interest, a well-defined simulation and modeling roadmap, and a timetable showing key milestones for each research area during the proposed life of the Center. The plan should include how to leverage existing computer science frameworks and science/engineering codes to more quickly bring up integrated simulation for their selected problem so more effort can be focused on the predictive science component. The approach should include a verification and validation plan and associated plan for how the required data is to be obtained.

(3) A one-page budget estimate and outline for the five years of the Center, including estimated costs for manpower and other resources, with supporting cost and burden rate data, and requirements for no-cost ASC Laboratory computational resources (e.g. time, processing elements, memory, archival storage, etc.). The MSC funding is estimated to ramp up, starting Government Fiscal Year 2008, as: $3.2M, $3.5M, $4.0M, $4.0M, and $4.0M (millions per year). Some discussion of the source of matching funds in the form of cash or direct cash equivalents of minimally 10%.

(4) A brief discussion of ideas for attracting US citizen graduate students and post docs, and associating them or involving them with the NNSA Laboratories (one page maximum).

(5) A brief list of ideas for interacting with the NNSA Laboratories (one page maximum).

(6) If appropriate, a list of potential collaborators from other universities and laboratories, including a BRIEF paragraph describing the nature of the contribution by the collaborator(s) (two pages maximum).

(7) While it is the intent of this program that the MSCs be largely centered within a single university, a proposing Center could fill a technical need by involving other universities. If so, the proposal will have to contain a clear plan for how the "prime" institution will manage the overall program with particular attention given to the partner university(ies). This should include a plan, not to exceed one page, for how the "prime" institution will manage adding or deleting partner universities and associated faculty and staff, as refocusing is needed or for non-performance. Clearly established roles and responsibilities of the "prime" and partner universities must be part of this plan.

(8) A one-page outline of the coordinated multidepartment/discipline structure of the Center. Include a list of senior endorsing officials (vice-chancellor, provost, etc.), heads of participating departments and key research personnel. Do not provide resumes or vitae, but a listing of sponsor names and contacts (and/or publication references) for 3-6 key related projects which are already completed or in process.

(9) Names, addresses, e-mail references, phone and facsimile numbers for a point of contact, the Principal Investigator, and a person authorized to execute any resulting contract (one page maximum).

Preliminary proposals should be submitted to the following:

Address for Commercial Courier:
University of California
Lawrence Livermore National Laboratory
Attention: Cindy Ehsan (B451, R2019)
Mail Code L-561
7000 East Avenue
Livermore, CA 94550

Address for Mailing:
University of California
Lawrence Livermore National Laboratory
Attention: Cindy Ehsan
Mail Code L-561
P.O. Box 5012
Livermore, CA 94551

Ten CDs of the preliminary proposals should be submitted. The document on disk should be in PDF and follow the document template provided in Appendix A herein. The CDs shall be labeled to include title of the proposed Center, institution name, Principal Investigator (PI)'s name, and date.

The preliminary proposals will be reviewed and evaluated by a panel of experts, including, but not limited to, NNSA ASC program and Laboratory personnel. The panel will provide feedback to all institutions that have submitted preliminary proposal(s). The evaluation criteria that will be used by the panel are as follows:

(1) Relevance and practicality of the proposed research plan, simulation and modeling methodology, and Center organization to the advancement of high-performance computing and PSAAP goals;

(2) Clarity of the multidisciplinary and disciplinary goals and objectives of PSAAP and the technical feasibility of the simulation sequences being coupled to accomplish them;

(3) Degree to which the various disciplines are integrated within the proposed Center;

(4) Degree to which the preliminary proposal incorporates a feasible and innovative plan for demonstrating agreement of simulation predictions with physical reality, including:

- Plan for verification and validation (V&V) of simulation capability.
- Plan for acquiring data for use in V&V effort.
- Plan for full-system science of prediction demonstration using the fully V&V'd simulation.

(5) Degree to which the models are integrated into an overarching computational framework;

(6) The capabilities, related experience, facilities, or techniques which are available for the work and are considered to be integral factors for achieving the objective(s) of the proposed work; and

(7) The validity of the requested ASC computing resources and capability of fully utilizing such resources.

The intent of the preliminary proposal review is to provide feedback to help the bidders in creating the strongest possible final proposals and to eliminate preliminary proposals that are not expected to be responsive in achieving the ASC PSAAP goals. At the time feedback is provided, institutions which have submitted responsive preliminary proposals will be encouraged to submit final, detailed proposals which will be evaluated for selection to receive MSC contracts.

Following the review of the responses to the Request for Expression of Interest (RFI), a competitive Request for Proposals (RFP) will be released.

The estimated MSC competition schedule is as follows:

- Preproposal Meeting – *May 16 -17, 2006*
- RFI issued – *May 26, 2006*
- Preliminary proposals due – *July 17, 2006*
- Review of preliminary proposals completed – *August 15, 2006*
- RFP issued– ***September 18, 2006***
- Final Proposals due – *November 30, 2006*

Questions and exchanges of information during the preliminary proposal process are encouraged. Please feel free to contact me by telephone at (925) 423-4732, or e-mail questions and comments to me at ehsan1@llnl.gov.

Regards,

Cindy Ehsan
University Procurement Representative
High Performance Computing Group

Additional PSAAP program statement and information may be found at http://www.llnl.gov/asci/alliances/psaap/.

For questions, contact:
Cindy Ehsan, Lawrence Livermore National Laboratory (ehsan1@llnl.gov)

For technical questions, contact:
Dick Watson, Lawrence Livermore National Laboratory (dwatson@llnl.gov)
Nelson M. Hoffman, Los Alamos National Laboratory (nmh@lanl.gov)
Tony Chen, Sandia National Laboratories (epchen@sandia.gov)
Thuc Hoang, National Nuclear Security Administration (thuc.hoang@nnsa.doe.gov)

Last modified June 2, 2006

Appendix A – Document Template

TABLE OF CONTENTS

1.	Executive Summary	NTE 1 page (insert bookmark)
2.	Technical and Scientific Approach	NTE 7 pages (insert bookmark)
3.	Budget Estimate	NTE 1 page (insert bookmark)
4.	Ideas on attracting US grad students & post docs	NTE 1 page (insert bookmark)
5.	Ideas on Interacting with NNSA Labs	NTE 1 page (insert bookmark)
6.	(Optional) List of potential collaborators	NTE 2 pages (insert bookmark)
7.	(Optional) Partnership Management Plan	NTE 1 page (insert bookmark)
8.	Outline of Center Management Structure	NTE 1 page (insert bookmark)
9.	Contact Information	NTE 1 page (insert bookmark)
10.	**Letter of Support from Vice President for Research**	**NTE 1 page (insert bookmark)**

NOTE:

- The enumerated sections above correspond to the respective requested informational sections called out on pages 3 and 4 of the RFI letter.
- "Insert bookmark" refers to the hotlink needed to go directly to that section of the electronic file that will be submitted to LLNL.
- "NTE" = "Not To Exceed"
- **A letter of support from the university VP for Research is required for each submission.**